

Crater Property in Two-Particle Bound States: When and Why

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Crater has shown that, for two particles (with masses m_1 and m_2) in a Coulombic bound state, the charge distribution is equal to the sum of the two charge distributions obtained by taking $m_1 \rightarrow \infty$ and $m_2 \rightarrow \infty$ respectively, while keeping the same Coulombic potential. We provide a simple scaling criterion to determine whether an arbitrary Hamiltonian possesses this property. In particular we show that, for a Coulombic system, fine structure corrections preserve this Crater property while two-particle relativistic corrections and/or hyperfine corrections may destroy it.

Recently, in an interesting paper in this journal [1], Crater discussed an unusual feature of charge densities for two-particle Coulombic bound states. Let $\rho(R; m_1, m_2)$ be the charge density of a two-particle bound state in a given potential $V(r) \equiv V(r_1 - r_2)$ in the center-of-mass coordinate system. Then Crater observed that, for a Coulombic potential the charge density satisfies the following relation:

$$\rho(R; m_1, m_2) = \lim_{m_2 \rightarrow \infty} \rho(R; m_1, m_2) + \lim_{m_1 \rightarrow \infty} \rho(R; m_1, m_2), \quad (1)$$

or, in Crater's own words, one can picture $\rho(R; m_1, m_2)$ "as equivalent to that produced by a particle of mass m_1 and charge e_1 , bound to a *fixed* center with charge e_2 plus that produced by a particle of mass m_2 and charge e_2 , bound to a *fixed* center with charge e_1 ," with the fixed center being the center of mass. Here and after this property will be referred to as the Crater property. Crater has shown in Ref. [1] that the Crater property holds for Coulombic potentials but not for generic potentials. In the real world, however, Coulombic potentials are often corrected by perturbations like fine/hyperfine structures and relativistic effects. It would be of interest to know what kind of corrections can be added to the Coulombic potential without destroying the Crater property. More generally, we would like to have a criterion to determine whether a given potential has the Crater property without explicitly solving the Schrödinger equation. The purpose of this paper is to provide answers to these questions.

Let us consider an eigenfunction $\psi(r; m_1, m_2)$ to the Schrödinger equation (in units $\hbar = 1$):

$$H(m_1, m_2)\psi(r; m_1, m_2) \equiv \left[\frac{-1}{2\mu} \frac{\partial^2}{\partial r_i^2} + V(r; m_1, m_2) \right] \psi(r; m_1, m_2) = E(m_1, m_2)\psi(r; m_1, m_2), \quad (2)$$

with $\mu = m_1 m_2 / M$ and $M = m_1 + m_2$. The charge density operator $\hat{\rho}(R)$ is defined as [1]

$$\hat{\rho}(R) = e_1 \delta^3(R - r_1) + e_2 \delta^3(R - r_2), \quad (3)$$

and the charge density $\rho(R; m_1, m_2)$ is its expectation value, which can easily be shown to be

$$\begin{aligned} \rho(R; m_1, m_2) &= \int d^3r |\psi(r; m_1, m_2)|^2 \hat{\rho}(R) \\ &= e_1 \left(\frac{M}{m_2} \right)^3 \left| \psi \left(\frac{M}{m_2} R; m_1, m_2 \right) \right|^2 + e_2 \left(\frac{M}{m_1} \right)^3 \left| \psi \left(\frac{M}{m_1} R; m_1, m_2 \right) \right|^2 \\ &= e_1 \left(\frac{m_1}{\mu} \right)^3 \left| \psi \left(\frac{m_1}{\mu} R; m_1, m_2 \right) \right|^2 + e_2 \left(\frac{m_2}{\mu} \right)^3 \left| \psi \left(\frac{m_2}{\mu} R; m_1, m_2 \right) \right|^2. \end{aligned} \quad (4)$$

Since the eigenfunction ψ , satisfying the normalization condition $\int d^3r |\psi|^2 = 1$, carries scaling dimension $[\text{length}]^{-3/2} = [\text{momentum}]^{3/2} = [\text{mass}]^{3/2}$ (with units $\hbar = c = 1$), it is always possible to rewrite $\psi(r; m_1, m_2)$ as

$$\psi(r; m_1, m_2) = \mu^{3/2} \tilde{\psi}(r; m_1, m_2), \quad (5)$$

where the rescaled eigenfunction $\tilde{\psi}(r; m_1, m_2)$ is a dimensionless function. Now consider the case when $\tilde{\psi}(r; m_1, m_2)$ has the following form:

$$\tilde{\psi}(r; m_1, m_2) \equiv \tilde{\psi}(\mu r), \quad (6)$$

which states that the dependences of $\tilde{\psi}$ on the location r and the masses $m_{1,2}$ always come through the combination $\mu r = m_1 m_2 r / (m_1 + m_2)$. Then $\psi(r; m_1, m_2) = \mu^{3/2} \tilde{\psi}(\mu r)$ and the charge density $\rho(R; m_1, m_2)$ in Eq. (4) becomes

$$\begin{aligned} \rho(R; m_1, m_2) &= e_1 \left(\frac{m_1}{\mu} \right)^3 \left| \mu^{3/2} \tilde{\psi} \left(\frac{m_1}{\mu} \mu R \right) \right|^2 + e_2 \left(\frac{m_2}{\mu} \right)^3 \left| \mu^{3/2} \tilde{\psi} \left(\frac{m_2}{\mu} \mu R \right) \right|^2 \\ &= e_1 m_1^3 \left| \tilde{\psi}(m_1 R) \right|^2 + e_2 m_2^3 \left| \tilde{\psi}(m_2 R) \right|^2 \\ &= \lim_{m_2 \rightarrow \infty} \rho(R; m_1, m_2) + \lim_{m_1 \rightarrow \infty} \rho(R; m_1, m_2), \end{aligned} \quad (7)$$

which is exactly the expression for the Crater property. In other words, the charge density exhibits the Crater property whenever the eigenfunction can be written as $\mu^{3/2} \tilde{\psi}(\mu r)$.

It is easy to translate the above scaling condition on the eigenfunction to a corresponding scaling condition on the Hamiltonian. Since the Hamiltonian $H(m_1, m_2)$ carries scaling dimension $[\text{mass}]^1$, it can always be rewritten as $\mu \tilde{H}(m_1, m_2)$, where \tilde{H} is a dimensionless function of $m_{1,2}$, as well as the relative coordinates r and the canonical momenta $-i\partial/\partial r$. It is straightforward to see that $\tilde{\psi}$ is a function of solely μr if and only if

$$\tilde{H}(m_1, m_2) = \tilde{\mathcal{H}} \left(\mu r, -i \frac{\partial}{\partial(\mu r)} \right) + \tilde{V}_0, \quad (8)$$

such that, up to an additive constant, the masses enter the Hamiltonian only through combinations μr and $-i(\partial/\partial(\mu r))$. The dimensionless constant \tilde{V}_0 , which may have arbitrary dependences on $m_{1,2}$, may shift the eigenvalues but does not affect the eigenfunctions.

We have shown that the charge density of an eigenfunction exhibits the Crater property if and only if the Hamiltonian can be written as

$$H = \mu \left[\tilde{\mathcal{H}} \left(\mu r, -i \frac{\partial}{\partial(\mu r)} \right) + \tilde{V}_0 \right], \quad (9)$$

which will be referred to as the scaling criterion. With this criterion one can easily determine if a particular potential exhibits the Crater property. For spinless Schrödinger systems, the kinetic term always satisfies the scaling criterion.

$$\frac{-1}{2\mu} \frac{\partial^2}{\partial r_i^2} = \mu \frac{-1}{2} \frac{\partial^2}{\partial(\mu r_i)^2}. \quad (10)$$

On the other hand, for analytic $V(r)$'s one can expand them in Laurent series and the scaling criterion is satisfied if and only if

$$V(r) = \sum_{k=-\infty}^{+\infty} a_k \mu^{k+1} r^k + \tilde{V}_0, \quad (11)$$

where a_k are mass independent coefficients. Of special interest is the case where the only non-vanishing a_k are those with $k = -1$ and -2 :

$$V(r) = \frac{a_{-1}}{r} + \frac{a_{-2}}{\mu r^2}, \quad (12)$$

which describes a Coulombic potential in three dimensions with $a_{-1} = e_1 e_2$ and $a_{-2} = \ell(\ell+1)/2$, *i.e.*, the case studied in Ref. [1]. Another interesting case is the “two-dimensional Coulombic potential”, *i.e.*, the logarithmic potential:

$$V(r) = e_1 e_2 \ln(r/r_0) = e_1 e_2 [\ln(\mu r) - \ln(\mu r_0)], \quad (13)$$

which can be seen to satisfy the scaling criterion by identifying the second term as \tilde{V}_0 .

As pointed out in Ref. [1], the Crater property is *not* a feature of potentials of generic r and mass dependences. Crater illustrated this point by studying the eigenfunctions of a simple harmonic potential and showed explicitly that $\rho(R; m_1, m_2)$, given by Eq. (4), is *not* the sum of $\lim_{m_2 \rightarrow \infty} \rho(R; m_1, m_2)$ and $\lim_{m_1 \rightarrow \infty} \rho(R; m_1, m_2)$, *i.e.*, the simple harmonic potential does not exhibit the Crater property. On the other hand, we can reproduce the same conclusion by just studying the scaling behavior of the simple harmonic potential:

$$V(r) = \frac{1}{2} \mu \omega^2 r^2, \quad (14)$$

which cannot be recast in a form conforming to criterion (9). As a result, the Crater property is not exhibited in simple harmonic potentials.

It is of interest to note that, for any potential $V(r) = \mu \tilde{V}(\mu r)$ satisfying the scaling criterion, including the fine structure corrections does not destroy the Crater property.

$$H_{mv} = \frac{-1}{8\mu^3 c^2} \left(\frac{\partial^2}{\partial r_i^2} \right)^2 = \mu \frac{-1}{8c^2} \left(\frac{\partial^2}{\partial (\mu r_i)^2} \right)^2, \quad (15)$$

$$H_{SO} = \frac{1}{\mu^2 c^2} \frac{1}{r} \frac{dV(r)}{dr} L \cdot S = \mu \frac{1}{c^2} \frac{1}{\mu r} \frac{d\tilde{V}(\mu r)}{d(\mu r)} L \cdot S, \quad (16)$$

$$H_D = \frac{1}{8\mu^2 c^2} \frac{d^2 V(r)}{dr_i^2} = \mu \frac{1}{8c^2} \frac{d^2 \tilde{V}(r)}{d(\mu r_i)^2}, \quad (17)$$

where H_{mv} , H_{SO} , and H_D stand for the relativistic mass variation term, the spin-orbit coupling term and the Darwin term, respectively. This may look miraculous but is actually nothing but a consequence of the fact that all these fine structure corrections come from the leading order expansion in the fine structure constant of the one-particle Dirac Hamiltonian with the same potential $V(r)$.

$$H = -i\alpha \cdot \frac{\partial}{\partial r} + \beta\mu + V(r) = \mu \left[-i\alpha \cdot \frac{\partial}{\partial (\mu r)} + \beta + \tilde{V}(\mu r) \right], \quad (18)$$

where α and β are the Dirac matrices. Since this one-particle Dirac Hamiltonian also satisfies the scaling criterion, the Crater property is preserved.

However, it is important to bear in mind that it is an approximation to describe a two-particle bound state by a one-particle Schrödinger or Dirac equation. Take, for example, the hyperfine correction, which for a Coulombic bound state is

$$H_{hf} = \frac{g_1 g_2 e_1 e_2}{3m_1 m_2} S_1 \cdot S_2 \delta^3(r) = \mu \left[\frac{\mu}{M} \right] \frac{g_1 g_2 e_1 e_2}{3} S_1 \cdot S_2 \delta^3(\mu r), \quad (19)$$

and the scaling criterion is violated by the outstanding factor of μ/M , where $M = m_1 + m_2$ is the total mass. Violations of the scaling criterion may also be due to two-particle relativistic effects. In the non-relativistic theory a two-particle problem can always be reduced to an effective one-particle problem in the relative coordinates, which decouple with the center-of-mass coordinates in the kinetic term:

$$\frac{1}{2m_1} \frac{\partial^2}{\partial r_1^2} + \frac{1}{2m_2} \frac{\partial^2}{\partial r_2^2} = \frac{1}{2M} \frac{\partial^2}{\partial R^2} + \frac{1}{2\mu} \frac{\partial^2}{\partial r^2}, \quad (20)$$

where R is the center of mass position $m_1 r_1 + m_2 r_2$, and r is the relative position $r_1 - r_2$. For a relativistic theory in general no such decomposition is possible, and the description of a two-particle problem by a one-particle equation is a good approximation only when one particle is much heavier than the other. Such treatments do not capture genuine two-particle effects, like the two-particle relativistic corrections and hyperfine corrections. These corrections in general do not satisfy the scaling criterion and one expects the Crater property to be violated by these corrections.

In passing, we note that the notion of Crater property can be generalized in a straightforward manner to any operator of the following form:

$$\mathcal{O}(R) = a \delta^3(R - r_1) + b \delta^3(R - r_2), \quad (21)$$

where a and b are arbitrary coefficients. This operator (R) may correspond to physically interesting objects for particular choices of a and b ; it is the charge density when $(a, b) = (e_1, e_2)$, the probability density of particle 1 and 2 when $(a, b) = (1, 0)$ and $(0, 1)$, respectively, and the mass density when $(a, b) = (m_1, m_2)$. Then the Hamiltonian or potential is said to exhibit the Crater property of charge/probability/mass distribution if and only if the charge/probability/mass distribution in the bound state of particle mass m_1 and m_2 is equivalent to the sum of the charge/probability/mass distributions produced in the limits $m_1 \rightarrow \infty$ and $m_2 \rightarrow \infty$. As before, all these Crater properties are guaranteed by the same scaling criterion (9).

In conclusion, we have provided a simple criterion to determine if the eigenfunctions of a given Hamiltonian have the Crater property. In particular, we have shown that neither the inclusions of fine structure corrections nor the switching from Schrödinger to Dirac formalism will destroy the Crater property. The author believes Crater must have foreseen the essential points of this paper — as in the conclusion of Ref. [1] he stated that “in general, the appearance of parameters in the potentials that are not dimensionless (in natural units) and do not depend on the reduced mass would not be of the correct type.” As a consequence, this paper may be regarded as a concrete realization of this observation.

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- [1] Horace W. Crater, “*An Unusual Feature of Charge Densities for Two-Particle Bound States*”, Am. J. Phys. **67** 739 (1999).